Spectral line broadening in stellar atmospheres

- Motivation:
- 1 Line broadening theory is a key ingredient in the construction of model atmospheres and synthetic spectra.
- 2 Useful temperature, density, abundance diagnostics.
- This lecture will discuss
- 1 The quasi-static line broadening theory applied to hydrogen line profiles. In particular will show that in the line wings the line opacity is well described by:

$$\alpha(\Delta\nu) \propto \Delta\nu^{-5/2}$$

2 applications to

white dwarfs: T_{eff} , $\log g$,

 δ Scuti stars: T_{eff} , [Fe/H], $v \sin i$.

- These lecture notes are based on:
- 1 Griem, H.R., Spectral line broadening by plasmas,
- 2 Sobel'man, I.I., Vainshtein, L.A., Yukov, E.A., Excitation of atoms and broadening of spectral lines,
- 3 Gray, D.F., The observation and analysis of stellar photospheres.

1. Spectral lines as a temperature, density and abundance diagnostic.



Figure 1: Spectral lines (H I Balmer, Ca II, Fe I, etc...) in white dwarfs and a giant F star (δ Scuti variable).

1. What is the microscopic situation ?

1.1: the motion of the test particle (an atom) and the perturbing particles is "classical".

1.2: trajectory is rectilinear.

1.3: the perturbation is adiabatic ... the encounter does not change the state of the atom



Figure 2: A test particle (H atom) is besieged by positively charged perturbers (Gray, *The Observation and Analysis of Stellar Photospheres*).



In addition, we may assume

1.3: that only the nearest particle contributes to line broadening ... binary interactions or **nearest-neighbor** hypothesis.

1.5: that the perturbers move slowly ... the **quasi-static** hypothesis.

1.6: or, in the **impact broadening** approximation, that spectral line shift are caused by instantaneous collisions.

2. What happens to a spectral line ?

2.1: assume that the energy levels involved in a line transition are perturbed (shifted) differently resulting in a net spectral line shift.

2.2: and describe that shift by:

$$\kappa = \Delta \omega = 2\pi \Delta \nu = C_n R^{-n}$$

n describes the form of the interaction field,

 C_n is an interaction constant, and

R is the separation between the atom and a single perturber.

2.3: For example, in a simple electrostatic field n = 2:

$$\Delta \omega = C_2 R^{-2} = C_2 \frac{F}{Ze} \qquad (C_2 \approx 1 \,\mathrm{cm}^2/\mathrm{s})$$

from which we can conclude that the **nearest neigh-bor** is responsible for the largest shift :



3. The nearest neighbor approximation ...

3.1: the field caused by the nearest particle is known

$$F(R)$$
 (or $\mathcal{E}(R)$)

3.2: what is the most probable distribution of this nearest perturber

knowing that there are

$$N = \left(\frac{4\pi}{3}R_0^3\right)^{-1}$$

such perturber per unit volume ? Find the probability that the nearest particle is in the range (R, R+dR):

 $P(\text{empty up to } R) \times P(\text{perturber inside } dV)$

where $dV = 4\pi R^2 dR$ is the volume of a shell at R.

3.3: The probabilities that the perturber be inside dV or not are simply:

$$\mathbf{P}(\text{perturber inside dV}) = \frac{dV}{V_0} = NdV$$

P(no perturber inside dV) = 1 - NdV

where V_0 is the volume occupied by a single perturber

$$V_0 = \frac{4\pi}{3}R_0^3 = \frac{1}{N}$$

Next, we evaluate the probability that the perturber is **not** within < R:

P(empty up to R+dR)

= $P(\text{empty up to } R) \times P(\text{no perturber inside } dV)$ that is:

 $P(\text{empty up to } R+dR) = P(\text{empty up to } R) \times (1-NdV)$ $\frac{P(\text{empty up to } R+dR) - P(\text{empty up to } R)}{P(\text{empty up to } R)} = -NdV$ $\frac{dP}{P} = -NdV$ $\ln P' \Big|_{1}^{P} = -NV' \Big|_{0}^{V}$

P(empty up to R) = $e^{-NV} = e^{-V/V_0}$

- 3.4 We now have the two ingredients required to describe the spatial distribution of a single perturber:
 - $W(R)dR = P(\text{empty up to } R) \times P(\text{perturber inside dV})$

$$W(R)dR = e^{-V/V_0} \frac{dV}{V_0}$$

Is that probability distribution **normalized** ?

$$\int_0^\infty W(R) dR = \int_0^\infty e^{-V/V_0} \frac{dV}{V_0} = \int_0^\infty e^{-u} du = 1$$

Recalling the density of perturber N

$$\frac{1}{V_0} = N$$

We now have the distance distribution for the **near-est neighbor**:

$$W(R)dR = e^{-\frac{4}{3}\pi R^3 N} 4\pi R^2 N dR = 3\left(\frac{R}{R_0}\right)^2 e^{-(R/R_0)^3} \frac{dR}{R_0}$$

W(R)

$$R_0$$
R

3.5 All distributions

distance to nearest neighbor W(R)dRresulting field at the atom W(F)dF

resulting line distribution $I(\Delta \omega) d\Delta \omega$

follow the same distribution law:

$$I(\Delta \omega)d\Delta \omega = W(F)dF = W(R)dR$$

where $\Delta \omega$ is measured from the line center ... So we may now calculate a normalized line distribution:

$$I(\Delta\omega) = W(R) \left| \frac{dR}{d\Delta\omega} \right|$$

For the frequency shift we have that in general:

$$\begin{split} \Delta \omega &= C_n R^{-n} \quad \to \quad R = C_n^{1/n} \Delta \omega^{-1/n} \\ \overline{\Delta \omega} &= C_n R_0^{-n} \quad \to \quad R_0 = C_n^{1/n} \overline{\Delta \omega}^{-1/n} \\ \left| \frac{dR}{d\Delta \omega} \right| &= \frac{C_n^{1/n}}{n} \Delta \omega^{-(n+1)/n} \\ I(\Delta \omega) &= \left(\frac{3}{R_0} \left(\frac{R}{R_0} \right)^2 e^{-(R/R_0)^3} \right) \left(\frac{C_n^{1/n}}{n} \Delta \omega^{-(n+1)/n} \right) \\ &= \left(\frac{3\overline{\Delta \omega}^{1/n}}{C_n^{1/n}} \left(\frac{\Delta \omega}{\overline{\Delta \omega}} \right)^{-2/n} e^{-(\Delta \omega/\overline{\Delta \omega})^{-3/n}} \right) \left(\frac{C_n^{1/n}}{n} \Delta \omega^{-(n+1)/n} \right) \end{split}$$

And re-grouping factors together and with a few cancellations, we have a more digestible:

$$I(\Delta\omega) = \frac{3}{n} \overline{\Delta\omega}^{3/n} \Delta\omega^{-(n+3)/n} e^{-(\Delta\omega/\overline{\Delta\omega})^{-3/n}}$$

The **nearest neighbor** approximation is only valid far in the line wing:

$$\Delta \omega >> \overline{\Delta \omega}$$

and the exponential factor ≈ 1 :

$$I(\Delta\omega) \approx \frac{3}{n} \overline{\Delta\omega}^{3/n} \Delta\omega^{-(n+3)/n}$$

Adopt a simple Coulomb interaction n = 2, and the result is a classic line-wing approximation for the calculation of line opacities in stellar atmospheres:

4. Holtsmark lifted the **nearest neighbor** restriction because it neglects the line centers.

The **nearest neighbor** at

 $R << R_0$

interacts strongly with the atomic energy levels (the "classical oscillator") and dominates the line wings at

$$\Delta \omega >> \overline{\Delta \omega}$$

Holtsmark theory includes a large number of distant neighbors

 $R \gtrsim R_0$

which dominate low fields ${\cal F}$ and the corresponding line center

$$\Delta\omega \leqslant \overline{\Delta\omega}$$

4.1 **Holtsmark theory** ... the field distribution in threedimension is the integral over a volume V of

$$W_0(\mathbf{F}) = \int \dots \int \int \delta(\mathbf{F} - \sum_{j=1}^n \mathbf{F}_j) P(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_n) d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \dots d^3 \mathbf{r}_n$$

The integral weighs in the many possibilities for $\mathbf{r}_1, \mathbf{r}_2, ... \mathbf{r}_n$ leading to the desired value of \mathbf{F} :

$$\mathbf{F} = \sum_{j=1}^{n} \mathbf{F}_{j}$$

since the particles are uncorrelated each set $\mathbf{r}_1, \mathbf{r}_2, ... \mathbf{r}_n$ has a probability:

$$P(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_n) = \frac{1}{V} \cdot \frac{1}{V} \dots \cdot \frac{1}{V} = \frac{1}{V^n}$$

where V is the volume containing all n particles, so

$$W_0(\mathbf{F}) = \frac{1}{V^n} \int \dots \int \int \delta(\mathbf{F} - \sum_{j=1}^n \mathbf{F}_j) \, d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \dots d^3 \mathbf{r}_n$$

Necessarily , the vector integral of the probability distribution over all field strengths is normalized

$$\int W_0(\mathbf{F}) d\mathbf{F} = 1$$

The Fourier transform $A(\mathbf{k})$ of this challenging integral is more amenable (after you're done, take the inverse transform to obtain $W_0(\mathbf{F})$). 4.2 Fourier transform of the field distribution $W_0(\mathbf{F})$.

$$A(\mathbf{k}) = \int e^{i\mathbf{k}\cdot\mathbf{F}} W_0(\mathbf{F}) d\mathbf{F}$$

Inserting our definition for the probability distribution $W_0(\mathbf{F})$:

$$A(\mathbf{k}) = \frac{1}{V^n} \int e^{i\mathbf{k}\cdot\mathbf{F}} \Big[\int \dots \int \int \delta(\mathbf{F} - \sum_{j=1}^n \mathbf{F}_j) \, d^3\mathbf{r}_1 d^3\mathbf{r}_2 \dots d^3\mathbf{r}_n \Big] d\mathbf{F}$$

and invert the order of integration:

$$\frac{1}{V^n} \int \dots \int \int \left[\int e^{i\mathbf{k}\cdot\mathbf{F}} \delta(\mathbf{F} - \sum_{j=1}^n \mathbf{F}_j) d\mathbf{F} \right] d^3\mathbf{r}_1 d^3\mathbf{r}_2 \dots d^3\mathbf{r}_n$$

 $A(\mathbf{k}) =$

after integrating over $d\mathbf{F}$

$$A(\mathbf{k}) = \frac{1}{V^n} \int \dots \int \int e^{i\mathbf{k} \cdot \sum_{j=1}^n \mathbf{F}_j} d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \dots d^3 \mathbf{r}_n$$

and each integral is independent and identical

$$A(\mathbf{k}) = \frac{1}{V^n} \int e^{i\mathbf{k}\cdot\mathbf{F}_1} d^3\mathbf{r}_1 \int e^{i\mathbf{k}\cdot\mathbf{F}_2} d^3\mathbf{r}_2 \dots \int e^{i\mathbf{k}\cdot\mathbf{F}_n} d^3\mathbf{r}_n$$
$$A(\mathbf{k}) = \left[\frac{1}{V} \int e^{i\mathbf{k}\cdot\mathbf{F}_1} d^3\mathbf{r}_1\right]^n = \left[\frac{1}{V} \int e^{i\mathbf{k}\cdot\mathbf{F}} d^3\mathbf{r}\right]^n$$

after dropping the subscript j.

4.3 Solving the Fourier transform $A(\mathbf{k})$:

$$A(\mathbf{k}) = \left[\frac{1}{V}\int e^{i\mathbf{k}\cdot\mathbf{F}} d^3\mathbf{r}\right]^n = I^n(\mathbf{k})$$

where

$$I(\mathbf{k}) = \frac{1}{V} \int e^{i\mathbf{k}\cdot\mathbf{F}} d^3\mathbf{r}$$

Lets define a few things in spherical geometry: (1) the dot product:

$$\mathbf{k}\cdot\mathbf{F}=kF\cos\theta$$

(2) the volume element:

$$d^3\mathbf{r} = r^2\sin\theta dr d\theta d\phi$$

(3) and happily integrate:

$$I(\mathbf{k}) = \frac{1}{V} \int r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta e^{ikF\cos\theta}$$

F = F(r) so wait before integrating r, go ahead with $\phi = [0, 2\pi]$, and substitute $u = kF \cos \theta$:

$$I(\mathbf{k}) = \frac{2\pi}{V} \int r^2 dr \int_{-kF}^{kF} \frac{du}{kF} e^{iu}$$

(in $e^{iu} = \cos u + i \sin u$, $\cos u$ is an "even" function and the integral vanishes, but $\sin u$ is "odd")

$$I(\mathbf{k}) = \frac{2\pi}{V} \int r^2 dr \left(\frac{\sin u}{kF}\right) \Big|_{-kF}^{kF} = \frac{4\pi}{V} \int r^2 dr \frac{\sin kF}{kF}$$

We complete the calculation of $I(\mathbf{k})$ with the integration over r:

$$I(\mathbf{k}) = \frac{4\pi}{V} \int r^2 dr \frac{\sin kF}{kF}$$
$$I(\mathbf{k}) = \frac{4\pi}{V} \int r^2 dr - \frac{4\pi}{V} \int r^2 dr + \frac{4\pi}{V} \int r^2 dr \frac{\sin kF}{kF}$$
$$V \text{ was taken large enough to include all } n \text{ perturber}$$

V was taken large enough to include all n perturber that affect the line profile, so r is integrated over V:

$$\begin{split} I(\mathbf{k}) &= 1 - \frac{4\pi}{V} \int r^2 dr + \frac{4\pi}{V} \int r^2 dr \frac{\sin kF}{kF} \\ I(\mathbf{k}) &= 1 - \frac{4\pi}{V} \int \left[1 - \frac{\sin kF}{kF} \right] r^2 dr \end{split}$$

Recall that the electric field F is given by:

$$F = \frac{Ze}{r^2}$$

so introduce the variable Y

$$\begin{split} Y &\equiv kF = \frac{kZe}{r^2} \to r^2 = \frac{kZe}{Y} \to dr = \frac{1}{2} \frac{(kZe)^{1/2}}{Y^{3/2}} \\ I(\mathbf{k}) &= 1 - \frac{4\pi}{V} \frac{1}{2} (kZe)^{3/2} \int_0^\infty \left[1 - \frac{\sin Y}{Y} \right] \frac{dY}{Y^{5/2}} \end{split}$$

This last definite integral is known (look it up in Abramowitz and Stegun!):

$$\int_0^\infty \left[1 - \frac{\sin Y}{Y}\right] \frac{dY}{Y^{5/2}} = \frac{4}{15} (2\pi)^{1/2}$$

And we finally have for $I(\mathbf{k})$:

$$I(\mathbf{k}) = 1 - \frac{4\pi}{V} \frac{1}{2} (kZe)^{3/2} \frac{4}{15} (2\pi)^{1/2}$$

simplify and regroup factors:

$$I(\mathbf{k}) = 1 - \frac{1}{V} \frac{4}{15} (2\pi)^{3/2} (Ze)^{3/2} k^{3/2}$$

The volume V is the volume chosen to contain all n perturber ... so the density of perturber is

$$N_p = \frac{n}{V} \longrightarrow \frac{1}{V} = \frac{N_p}{n}$$
$$I(\mathbf{k}) = 1 - \frac{1}{n} \frac{4}{15} (2\pi)^{3/2} (Ze)^{3/2} N_p k^{3/2}$$

The quantity F_0 is now defined as the "normal field strength":

$$\frac{4}{15}(2\pi)^{3/2}(Ze)^{3/2}N_p \equiv F_0^{3/2} \quad \to \quad F_0 = 2\pi(4/15)^{2/3}ZeN_p^{2/3}$$

$$F_0 = 2.603 Ze N_p^{2/3}$$

Note that you could directly estimate $F_0 = Ze/R_0^2$ using $N_p = (4\pi/3)R_0^3$ and obtain

$$F_0 = 2.595 Ze N_p^{2/3}$$

Close enough, but not exact.

Anyway we can now complete our estimate of the Fourier transform of $W_0(\mathbf{F})$:

$$A(\mathbf{k}) = I^{n}(\mathbf{k}) = \left[1 - \frac{1}{n}F_{0}^{3/2}k^{3/2}\right]^{n}$$

Take n as large as you want! the limit is very useful:

$$\lim_{n \to \infty} \left[1 - \frac{1}{n} x \right]^n = e^{-x}$$

So that $A(\mathbf{k})$ is isotropic and a simple exponential:

$$A(\mathbf{k}) = e^{-F_0^{3/2}k^{3/2}} = e^{-(kF_0)^{3/2}}$$

4.4 We are now ready to determine the field distribution $W_0(\mathbf{F})$ by taking the inverse transform (in threedimensions):

$$W_0(\mathbf{F}) = \frac{1}{(2\pi)^3} \int e^{-i\mathbf{k}\cdot\mathbf{F}} A(\mathbf{k}) d\mathbf{k}$$

We're again integrating in 3D so we wont repeat everything, but note that:

$$\mathbf{k} \cdot \mathbf{F} = kF \cos \theta$$
$$d\mathbf{k} = 2\pi k^2 dk \sin \theta d\theta$$

and the integration over θ is quickly performed, leaving the integration over k

$$W_0(\mathbf{F}) = \frac{1}{(2\pi)^2} \int A(\mathbf{k}) \frac{2\sin(kF)}{kF} k^2 dk$$

And simplifying a little:

$$W_0(\mathbf{F}) = \frac{1}{(2\pi)^2} \frac{2}{F} \int A(\mathbf{k}) \sin(kF) k dk$$

We do expect the distribution to be isotropic (no preferred directions in space), so we can now estimate the probability W(F) inside the shell $4\pi F^2$:

$$W(F) = 4\pi F^2 W_0(\mathbf{F}) = 4\pi F^2 \frac{1}{(2\pi)^2} \frac{2}{F} \int A(\mathbf{k}) \sin(kF) k dk$$
$$W(F) = \frac{2}{\pi} F \int A(\mathbf{k}) \sin(kF) k dk$$

And recall our result for the Fourier transform:

$$A(\mathbf{k}) = e^{-(kF_0)^{3/2}}$$
$$W(F) = \frac{2}{\pi}F \int e^{-(kF_0)^{3/2}} \sin(kF)kdk$$

With one last change of variable:

$$x = kF_0$$

$$W(F) = \frac{2}{\pi}F \int e^{-x^{3/2}} \sin(x\frac{F}{F_0})\frac{x}{F_0}\frac{dx}{F_0}$$

and define the dimensionless variable $\beta = F/F_0$:

$$W(F) = \frac{2}{\pi} \frac{\beta}{F_0} \int e^{-x^{3/2}} \sin(x\beta) x \, dx$$

4.5 And FINALLY, introduce the **Holtsmark distribution** $H(\beta)$:

$$H(\beta)d\beta = W(F)dF$$

and since $\beta = F/F_0$:

$$H(\beta) = F_0 W(F)$$
$$H(\beta) = \frac{2}{\pi} \beta \int_0^\infty e^{-x^{3/2}} \sin(x\beta) x \, dx$$

How does one integrate this? Numerically! For $\beta >>$:

A general solution for $\beta >>$ can be obtained by expanding the integrand in a series and obtain:

$$H(\beta) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n!} \Gamma(\frac{3n+4}{2}) \sin(\frac{3n\pi}{4}) \beta^{-(3n+2)/2}$$

and retaining only the n = 1 term of the series:

$$H(\beta) \approx 1.496 \beta^{-5/2} \propto \Delta \omega^{-5/2}$$

in agreement with the **nearest neighbor**:

$$H(\beta) \approx 1.5 \beta^{-5/2} \propto \Delta \omega^{-5/2}$$

But we did not exclude weak fields, so we expect the distribution to be correct everywhere in the line pro-

4.6 How does **Holtsmark theory** compare to recent

 $\Delta \nu(s^{-1})$ In red, the line wing behavior, in blue, the Doppler profile, with adashed line, the **Holtsmark theory**, and with a full line, the full impact/Holtsmark theory of Vidal, Cooper, and Smith (1973).

5.1 White dwarfs. Computed using Vennes & Kawka codes (employs Lemke and Vidal, Cooper & Smith line profiles based on **Holtsmark theory** in the line wings, and impact broadening theory in the center).

Figure 3: Temperature and gravity diagnostics for the low-mass white dwarf LP400-22 ($M_V = 9.1$).

Figure 4: Temperature and gravity diagnostics for the high-mass white dwarf NLTT 44986 ($M_V = 14.5$).

Figure 5: H-R diagram for white dwarfs built using temperature and gravity diagnostics based on Balmer line profiles.

5.2 δ Scuti stars. Computed using Kurucz's ATLAS codes (employs **Holtsmark theory**).

Figure 6: Atmospheric diagnostics for a δ Scuti star.

Figure 7: Atmospheric diagnostics for a δ Scuti star. Note the rotationally broadened line profiles.

Figure 8: H-R diagram for a sample of variable giants and sub-giants built using line profile diagnostics.